.

Heat flow in chains driven by thermal noise

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Abstract

We consider the large deviation function for a classical harmonic chain composed of N particles driven at the end points by heat reservoirs, first derived in the quantum regime by Saito and Dhar [1] and in the classical regime by Saito and Dhar [2] and Kundu et al. [3]. Within a Langevin description we perform this calculation on the basis of a standard path integral calculation in Fourier space. The cumulant generating function yielding the large deviation function is given in terms of a transmission Green's function and is consistent with the fluctuation theorem. We find a simple expression for the tails of the heat distribution which turn out to decay exponentially. We, moreover, consider an extension of a single particle model suggested by Derrida and Brunet [4] and discuss the two-particle case. We also discuss the limit for large N and present a closed expression for the cumulant generating function. Finally, we present a derivation of the fluctuation theorem on the basis of a Fokker-Planck description. This result is not restricted to the harmonic case but is valid for a general interaction potential between the particles.

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I. INTRODUCTION

There is a current interest in the thermodynamics and statistical mechanics of fluctuating systems in contact with heat reservoirs and driven by external forces. The current focus stems from the recent possibility of direct manipulation of nano-systems and bio-molecules. These techniques permit direct experimental access to the probability distribution functions for the work or for the heat exchanged with the environment [5–15]. These methods have also yielded access to the experimental verification of the recent fluctuation theorems which relate the probability of observing entropy-generated trajectories with that of observing entropy-consuming trajectories [16–33].

In recent works we studied the motion of a Brownian particle in a general potential with a view to the distribution function for the heat exchange with the surroundings [34] and a single bound Brownian particle driven by two heat reservoirs [35]. In the present paper we consider the harmonic chain driven by heat reservoirs at temperatures T_1 and T_N [36, 42–49]. Here the distribution of positions and momenta is given by a Gaussian form with a correlation matrix with elements given by the static position and momentum correlations [36].

Owing to the current interest in fluctuation theorems the linear chain has recently been addressed again by Saito and Dhar [2] and by Kundu et al. [3]; see also [1] for a treatment in the quantum regime. Using a path integral formulation, Fourier series, and analyzing the resulting energy transmission matrices, these authors derive an expression for the cumulant generating function, in the following denoted CGF, for the heat transfer in terms of a transmission Green's function $T(\omega)$. The large deviation function for the heat transfer, denoted LDF, then follows by a Legendre transformation of the CGF; for definitions, see later. The expression is in accordance with the fluctuation theorem [17, 19, 21, 23–26].

In the present paper we consider four issues: i) the CGF for the harmonic chain, ii) the LDF for the chain and the exponential tails in the heat distribution, iii) the CGF for an extension of a model by Derrida and Brunet [4], iv) the CGF for the harmonic chain in the large N limit, where N is the number of particles, and v) a derivation of the fluctuation theorem on the basis of a Fokker-Planck description.

For the purpose of the analysis in ii) - iv) we have within a Langevin scheme performed a calculation of the CGF, including explicit expressions for the transmission Green function.

At the technical level we, moreover, unlike Kundu et al. [3], make use of Fourier transforms throughout the calculation and diagonalize explicitly $T(\omega)$ expressing the CGF in terms of the eigenvalues. For the benefit of the reader and the continuity of the paper we have chosen to include this analysis in the main part of the paper.

We discuss the tails in the heat distribution and exemplify this feature both for the extended Derrida-Brunet model and the N particle chain. We consider the CGF and LDF for an extension of a single particle model suggested by Derrida and Brunet [4] and the CGF in the two-particle case. We, moreover, analyze the asymptotic large N limit and present a closed expression for the CGF.

Finally, as a related and more formal issue we present a derivation of the fluctuation theorem on the basis of a Fokker-Planck description of a chain. As a bonus we are able to prove that the fluctuation theorem holds for chains with general interaction potentials and with several heath baths at different temperatures.

For reference we present below the results of Saito and Dhar [2] and Kundu et al. [3], also presented in the present paper. Denoting the model-dependent transmission Greens function by $T(\omega)$, the CGF $\mu(\lambda)$ for the characteristic function for the transferred heat $Q(t)$ in the time interval t, is given by the following expressions:

$$\langle \exp(\lambda Q(t)) \rangle = \exp(t\mu(\lambda)), \tag{1.1}$$

$$\mu(\lambda) = -\frac{1}{2}\int \frac{d\omega}{2\pi}\ln[1 + T(\omega)f(\lambda)], \tag{1.2}$$

$$f(\lambda) = T_1 T_N \lambda(1/T_1 - 1/T_N - \lambda). \tag{1.3}$$

Here T_1 and T_N denote the reservoir temperatures and the form of $f(\lambda)$ ensures the validity of the fluctuation theorem

$$\mu(\lambda) = \mu(1/T_1 - 1/T_N - \lambda). \tag{1.4}$$

As a new result we present below the CGF in the asymptotic large N limit. Here Γ denotes the reservoir damping and κ the spring constant. The CGF is given by

$$\mu(\lambda) = -\int_0^\pi \frac{dp}{2\pi}\sqrt{\kappa}\cos(p/2)\ln\left[1 + \frac{8\Gamma\kappa^{-1/2}\sin(p/2)\sin(p)f(\lambda)}{1 + 4(\Gamma^2/\kappa)\sin^2(p/2)}\right]. \tag{1.5}$$

Finally, we note that the mathematical background for the present paper is provided by large deviation theory, see Refs. [37–41].

The paper is organized in the following manner. In Sec. II we present the harmonic chain. In Sec. III we set up the necessary analysis. In Sec. IV we present a derivation of the CGF. The general properties of such a function are discussed in Sec. V, where we also consider the tails of the heat distribution, the specific cases of a bound Brownian particle, a two-particle chain, and the large N limit. In Sec. VI we discuss a generalization of the fluctuation theorem. In Sec. VII we present a summary and a conclusion.

II. HARMONIC CHAIN

The dynamics of a unit mass harmonic chain composed of N particles and, moreover, attached to a wall or substrate, is governed by the Hamiltonian

$$H = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + \frac{\kappa}{2}\sum_{n=1}^{N-1}(u_n - u_{n+1})^2 + \frac{\kappa}{2}(u_1^2 + u_N^2), \tag{2.1}$$

where u_n and p_n denotes displacements and momenta, respectively; κ is the spring constant. The equation of motion for the bulk particles and the end particles driven by the heat reservoirs at temperatures T_1 and T_N with associated damping Γ are given by

$$\frac{du_n}{dt} = p_n, \tag{2.2}$$

$$\frac{dp_n}{dt} = \kappa(u_{n+1} + u_{n-1} - 2u_n), \quad n = 2, \cdots N - 1, \tag{2.3}$$

$$\frac{dp_1}{dt} = -\Gamma p_1 + \kappa(u_2 - 2u_1) + \xi_1, \tag{2.4}$$

$$\frac{dp_N}{dt} = -\Gamma p_N + \kappa(u_{N-1} - 2u_N) + \xi_N, \tag{2.5}$$

with noise correlations and strengths

$$\langle \xi_1(t)\xi_1(t')\rangle = \Delta_1 \delta(t - t'), \tag{2.6}$$

$$\langle \xi_N(t)\xi_N(t')\rangle = \Delta_N \delta(t - t'), \tag{2.7}$$

$$\Delta_1 = 2\Gamma T_1, \tag{2.8}$$

$$\Delta_N = 2\Gamma T_N; \tag{2.9}$$

in equilibrium $\Delta_1 = \Delta_N = \Delta$ and detailed balance implies $\Delta = 2\Gamma T$, where T is the common temperature of the reservoirs.

Focussing on the reservoir at temperature T_1 the fluctuating force is given by $-\Gamma p_1 + \xi_1$ and, correspondingly, the rate of work or heat flux has the form, denoting $Q \equiv Q_1$,

$$\frac{dQ}{dt} = p_1(-\Gamma p_1 + \xi_1). \tag{2.10}$$

The central quantity in the analysis is, however, the total heat transmitted during a finite time interval t, i.e.,

$$Q(t) = \int_0^t d\tau\, p_1(\tau)(-\Gamma p_1(\tau) + \xi_1(\tau)); \tag{2.11}$$

note that strictly speaking only the time scaled heat $Q(t)/t$ has large deviation properties, see e.g. Refs. [37, 41].

The heat $Q(t)$ is fluctuating and the issue is to determine its probability distribution $P(Q,t) = \langle \delta(Q - Q(t)) \rangle$; here $\langle \cdots \rangle$ denotes an average with respect to ξ_1 and ξ_N. In terms of the characteristic function $\langle \exp(\lambda Q(t) \rangle$ we have by a Laplace transform [55]

$$P(Q,t) = \int_{-i\infty}^{i\infty} \frac{d\lambda}{2\pi i} e^{-\lambda Q} \langle e^{\lambda Q(t)} \rangle. \tag{2.12}$$

The chain attached to the substrate at the ends and driven by heat reservoirs is depicted in Fig. 1.

III. ANALYSIS

The heat reservoirs drive the chain into a stationary state. Since the heat is transported ballistically the only damping mechanism is associated with the heat reservoirs and the only time scale is given by $1/\Gamma$. Consequently, at long times compared with $1/\Gamma$ we can neglect the initial preparation of the chain and analyze the problems in terms of Fourier transforms. Thus introducing the Fourier transform

$$u_n(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} u_n(\omega), \tag{3.1}$$

the equations of motion (2.2) to (2.5) and noise correlations (2.6) to (2.7) take the form

$$\sum_{m=1}^{N} G_{nm}^{-1}(\omega) u_m(\omega) = \delta_{n1}\xi_1(\omega) + \delta_{nN}\xi_N(\omega), \tag{3.2}$$

$$\langle \xi_1(\omega)\xi_1(\omega') \rangle = 2\pi\Delta_1\delta(\omega + \omega'), \tag{3.3}$$

$$\langle \xi_N(\omega)\xi_N(\omega') \rangle = 2\pi\Delta_N\delta(\omega + \omega'). \tag{3.4}$$

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Here the inverse Green's function $G_{nm}^{-1}(\omega)$ is a symmetrical tridiagonal matrix with elements

$$G_{11}^{-1}(\omega) = G_{NN}^{-1}(\omega) = \Omega, \tag{3.5}$$

$$G_{nn}^{-1}(\omega) = \widetilde{\Omega}, \quad n = 2, \cdots N-1, \tag{3.6}$$

$$G_{nn+1}^{-1}(\omega) = G_{nn-1}^{-1}(\omega) = -\kappa, \tag{3.7}$$

where

$$\Omega = -\omega^2 + 2\kappa - i\Gamma\omega, \tag{3.8}$$

$$\widetilde{\Omega} = -\omega^2 + 2\kappa; \tag{3.9}$$

note that for a free chain we have $\Omega = -\omega^2 + \kappa - i\Gamma\omega$.

Propagating bulk solutions have the form

$$u_n(\omega) = A\exp(ipn) + B\exp(-ipn), \tag{3.10}$$

$$\omega^2 = 4\kappa\sin^2(p/2), \tag{3.11}$$

where p is confined to the first Brillouin zone $|p| < \pi$ and, correspondingly, $|\omega| < 2\sqrt{\kappa}$. Imposing the noisy drive we readily determine the coefficients A and B and infer the solutions

$$u_n(\omega) = G_{n1}(\omega)\xi_1(\omega) + G_{nN}(\omega)\xi_N(\omega), \quad p_n(\omega) = (-i\omega)u_n(\omega), \tag{3.12}$$

where the Green function components are given by

$$G_{n1}(\omega) = \frac{\Omega\sin(N-n)p - \kappa\sin(N-n-1)p}{D(\omega)}, \tag{3.13}$$

$$G_{nN}(\omega) = \frac{\Omega\sin(n-1)p - \kappa\sin(n-2)p}{D(\omega)}, \tag{3.14}$$

$$D(\omega) = \Omega^2\sin(N-1)p - 2\kappa\Omega\sin(N-2)p + \kappa^2\sin(N-3)p. \tag{3.15}$$

The displacement u_n is thus driven by stochastically excited lattice waves (phonons) propagating towards the site from the end points; $D(\omega) = 0$ yield the damped mode spectrum. Also, from the definition of $G_{nm}^{-1}(\omega)$ we deduce the relationship $G_{nm}^{-1}(\omega) - G_{nm}^{-1}(-\omega) = -2i\omega\Gamma\delta_{nm}(\delta_{n1} + \delta_{nN})$ and by multiplication the Schwinger identity [50]

$$G_{nm}(\omega) - G_{nm}(\omega)^* = 2i\omega\Gamma[G_{n1}(\omega)G_{1m}(\omega)^* + G_{nN}(\omega)G_{Nm}(\omega)^*]. \tag{3.16}$$

In the absence of the heat reservoirs energy is conserved, i.e., $dH/dt = 0$, where H is given by (2.1). Coupling the reservoirs to the chain we have $dH/dt = dQ_1/dt + dQ_N/dt$,

where dQ_N/dt is the heat flux from the reservoir at temperature T_N. Averaging we have for the mean heat fluxes $\langle dQ_1/dt \rangle = -\langle dQ_N/dt \rangle$, expressing the energy balance; the mean input flux at $n = 1$ is equal to the mean output flux at $n = N$.

Using (2.10), inserting (3.12), averaging over the noises (3.3) and (3.4), using the properties of the Green's function (3.13) and (3.14), and the identity (3.16), we obtain for the mean transferred heat in time t

$$\langle Q(t) \rangle = t(\Delta_1 - \Delta_N)\Gamma \int \frac{d\omega}{2\pi} \omega^2 |G_{1N}(\omega)|^2. \tag{3.17}$$

Here the central model dependent quantity is the end-to-end Greens function $G_{1N}(\omega)$; we note that the mean heat vanishes for $\Delta_1 = \Delta_N$. We also note that the transferred mean heat rate $\bar{q} = \langle Q \rangle / t$ is given by

$$\bar{q} = \Gamma(T_1 - \langle p_1^2 \rangle); \tag{3.18}$$

see Ref. [36]. Here $\langle p_1^2 \rangle$ is the average kinetic temperature of the first particle in the steady state; note that in equilibrium $\bar{q} = 0$ and $\langle p_1^2 \rangle = T_1$ in accordance with the equipartition theorem [51]. The relation (3.18) follows from (3.17) by inserting the Greens function solution of the equations of motion and using the identity (3.16).

The expression (3.18) also follows from the equivalent Fokker-Planck approach to the harmonic chain which we discuss below. Considering the definition of the n-th moment of the heat transfer in time t

$$\langle Q^n(t) \rangle = \int dQ du dp \, Q^n P(u, p, Q, t), \tag{3.19}$$

and referring to (6.6) in Sec. VI, the Fokker-Planck equation for the joint distribution $P(u, p, Q, t)$ in the case of two reservoirs implies

$$\frac{d\langle Q^n \rangle}{dt} = \Gamma n \langle (T_1 - p_1^2)Q^{n-1} \rangle + \Gamma n(n-1)T_1 \langle p_1^2 Q^{n-2} \rangle. \tag{3.20}$$

These equations of motion are part of a hierarchy relating the n-th moment to correlations of the lower moments with $\langle p_1^2 \rangle$ and have to be completed by equations of motions for the correlations $\langle p_1^2 Q^{n-2} \rangle$. Without further assumptions this hierarchy will in general not terminate and simply represents a reformulation. We note, however, that for the first moment for $n = 1$ the second term in (3.20) vanishes and we obtain a closed equation yielding (3.18).

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For the fluctuating heat transferred in time t we obtain, using (2.11) and inserting (3.12), the expression

$$Q(t) = \int \frac{d\omega}{2\pi} \frac{d\omega'}{2\pi} F(\omega - \omega') \left(\xi_1(\omega) \ \xi_N(\omega) \right) M(\omega, \omega') \begin{pmatrix} \xi_1(-\omega') \\ \xi_N(-\omega') \end{pmatrix}. \tag{3.21}$$

The heat transfer is a fluctuating quantity depending bilinearly on the reservoir noises ξ_1 and ξ_N. The matrix elements in the symmetrical form (3.21) are given by

$$M_{11}(\omega, \omega') = -\Gamma A(\omega) A(\omega')^* + (1/2)(A(\omega) + A(\omega')^*), \tag{3.22}$$

$$M_{22}(\omega, \omega') = -\Gamma B(\omega) B(\omega')^*, \tag{3.23}$$

$$M_{12}(\omega, \omega') = -\Gamma A(\omega) B(\omega')^* + (1/2)B(\omega')^*, \tag{3.24}$$

$$M_{21}(\omega, \omega') = -\Gamma B(\omega) A(\omega')^* + (1/2)B(\omega), \tag{3.25}$$

where we have introduced the notation

$$A(\omega) = -i\omega G_{11}(\omega), \tag{3.26}$$

$$B(\omega) = -i\omega G_{1N}(\omega); \tag{3.27}$$

we note that (3.16) implies

$$A(\omega) + A(\omega)^* = 2\Gamma[|A(\omega)|^2 + |B(\omega)|^2]. \tag{3.28}$$

The dependence on the transfer time t is embodied in the function

$$F(\omega) = 2e^{-i\omega t/2} \frac{\sin(\omega t/2)}{\omega}. \tag{3.29}$$

For later purposes we also note that

$$F(0) = t, \tag{3.30}$$

$$|F(\omega)|^2 = 2\pi t \delta(\omega) \quad \text{for large } t. \tag{3.31}$$

At this stage our calculation differs from Kundu et al. [3] in that we use a Fourier transform instead of a Fourier series in the expression (3.21) for the fluctuating heat. The dependence on the transfer time t is then incorporated in the function $F(\omega)$.

IV. LARGE DEVIATION FUNCTION

For large t the mean heat $\langle Q(t) \rangle$ given by (3.17) grows linearly with time. Analyzing the higher cumulants $\langle Q(t)^n \rangle_c$, i.e., $\langle Q(t)^2 \rangle_c = \langle Q(t)^2 \rangle - \langle Q(t) \rangle^2$, etc., by averaging over the noise and applying Wick's theorem [52], it also follows that they likewise increase linearly with time, i.e., $\langle Q(t)^n \rangle_c \sim t$ for large t. We thus infer from the cumulant expansion of the characteristic function [51],

$$\langle \exp(\lambda Q(t)) \rangle = \exp \left(\sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \langle Q(t)^n \rangle_c \right), \tag{4.1}$$

that for large t

$$\langle \exp(\lambda Q(t)) \rangle = \exp(t\mu(\lambda)), \tag{4.2}$$

where $\mu(\lambda)$ is the cumulant generating function, denoted CGF.

The CGF characterizes the long time heat distribution. From the cumulant expansion (4.1) we obtain the relationship

$$\left(\frac{d^n \mu(\lambda)}{d\lambda^n} \right)_{\lambda=0} = \frac{\langle Q(t)^n \rangle_c}{t}. \tag{4.3}$$

Here the definition (4.2) for $\lambda = 0$ implies

$$\mu(0) = 0. \tag{4.4}$$

In case the fluctuation theorem is valid we, moreover, have the symmetry

$$\mu(\lambda) = \mu(1/T_1 - 1/T_N - \lambda). \tag{4.5}$$

Turning to the evaluation of $\mu(\lambda)$ we average $\exp(\lambda Q(t))$ with respect to the noises ξ_1 and ξ_N. In matrix form the Gaussian noise distribution has the form

$$P(\xi) \propto \exp \left(-\frac{1}{2} \int \frac{d\omega \, d\omega'}{2\pi \, 2\pi} \tilde{\xi}(\omega) \Delta^{-1}(\omega - \omega') \xi(-\omega') \right), \tag{4.6}$$

where $\tilde{\xi}(\omega) = (\xi_1(\omega), \xi_N(\omega))$ and the inverse noise matrix is given by

$$\Delta^{-1}(\omega - \omega') = \begin{pmatrix} \Delta_1^{-1} & 0 \\ 0 & \Delta_N^{-1} \end{pmatrix} \delta(\omega - \omega'). \tag{4.7}$$

Noting from (3.21) that $Q(t)$ is bilinear in ξ and using the identities [52]

$$\langle \exp(-(1/2)\tilde{\xi}B\xi)\rangle = \det(I + \Delta B)^{-1/2}, \tag{4.8}$$

$$\det(A) = \exp(\operatorname{Tr}\ln(A)), \tag{4.9}$$

we obtain for the CGF

$$\mu(\lambda) = -\frac{1}{2t}\operatorname{Tr}\ln(I - 2\lambda\Delta FM). \tag{4.10}$$

In the remaining part of this section the present calculation differs from Kundu et al. [3] in that we owing to the nondiagonal character of F must expand μ in order to implement the large t limit. Thus expanding the log according to $\ln(1 + x) = \sum_{n=1}(-1)^{n+1}x^n/n$ and tracing term by term we have

$$\mu(\lambda) = -\frac{1}{2t}\sum_{n=1}\frac{(-1)^{n+1}}{n}(-2\lambda)^n\operatorname{Tr}(\Delta FM)^n, \tag{4.11}$$

and the issue is to determine $\operatorname{Tr}(\Delta FM)^n$ and complete the sum. From (3.21) we obtain

$$\operatorname{Tr}(\Delta FM)^n = \int\prod_{k=1}^{n}\frac{d\omega_k}{2\pi}F(\omega_k - \omega_{k+1})\operatorname{Tr}\left(\prod_{k=1}^{n}\Delta M(\omega_k, \omega_{k+1})\right), \tag{4.12}$$

where $\omega_{n+1} = \omega_1$. Inserting (3.29) we notice that since $\sum_{k=1}^{n}(\omega_k - \omega_{k+1}) = 0$ the exponential factors in the product of F functions combine yielding a unit factor. We thus only have to retain the sine part, i.e., $F(\omega) \to 2\sin(\omega t/2)/\omega$. Using (3.30) and (3.31) we have for $n = 1, 2$

$$\operatorname{Tr}(\Delta FM) = t\int\frac{d\omega}{2\pi}\operatorname{Tr}(\Delta M(\omega, \omega)), \tag{4.13}$$

$$\operatorname{Tr}(\Delta FM)^2 = t\int\frac{d\omega}{2\pi}\operatorname{Tr}(\Delta M(\omega, \omega)\Delta M(\omega, \omega)). \tag{4.14}$$

For large t the function $F(\omega)$ oscillates rapidly as a function of ω and we have approximately $\omega_1 \sim \omega_2 \cdots \sim \omega_n$, i.e., the effective integration range in ω space is confined to the domain $\omega_1 = \omega_2 = \cdots = \omega_n$ and only one ω integration remains. Using $\int(d\omega/2\pi)F(\omega) = 1$ inspection readily yields

$$\operatorname{Tr}(\Delta FM)^n = t\int\frac{d\omega}{2\pi}\operatorname{Tr}((\Delta M(\omega, \omega)^n), \tag{4.15}$$

and the CGF takes the form

$$\mu(\lambda) = -\frac{1}{2}\sum_{n=1}\frac{(-1)^{n+1}}{n}(-2\lambda)^n\int\frac{d\omega}{2\pi}\operatorname{Tr}((\Delta M(\omega, \omega)^n). \tag{4.16}$$

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In order to complete the calculation we diagonalize the two-by-two matrix ΔM. Denoting the eigenvalues by $\alpha_+(\omega)$ and $\alpha_+(\omega)$ we have $\text{Tr}((\Delta M(\omega,\omega))^n) = \alpha_+(\omega)^n + \alpha_-(\omega)^n$ and reconstructing the log we obtain for $\mu(\lambda)$

$$\mu(\lambda) = -\frac{1}{2}\int \frac{d\omega}{2\pi}[\ln(1 - 2\lambda\alpha_+(\omega)) + \ln(1 - 2\lambda\alpha_-(\omega))], \tag{4.17}$$

The eigenvalues $\alpha_+(\omega)$ and $\alpha_+(\omega)$ are determined by the condition $\det(\Delta M - \alpha I) = 0$, i.e.,

$$\begin{vmatrix} \Delta_1 M_{11}(\omega,\omega) - \alpha(\omega) & \Delta_1 M_{12}(\omega,\omega) \\ \Delta_N M_{21}(\omega,\omega) & \Delta_N M_{22}(\omega,\omega) - \alpha(\omega) \end{vmatrix} = 0, \tag{4.18}$$

yielding the quadratic equation

$$\alpha^2 - \alpha(\Delta_1 M_{11} + \Delta_N M_{22}) + \Delta_1\Delta_N(M_{11}M_{22} - M_{12}M_{21}) = 0, \tag{4.19}$$

with roots α_+ and α_-. In particular

$$\alpha_+ + \alpha_- = \Delta_1 M_{11} + \Delta_N M_{22}, \tag{4.20}$$

$$\alpha_+\alpha_- = \Delta_1\Delta_N(M_{11}M_{22} - M_{12}M_{21}). \tag{4.21}$$

Using the identity (3.28) we obtain the reduced expressions

$$M_{11}(\omega,\omega) = -M_{22}(\omega,\omega) = \Gamma|B(\omega)|^2, \tag{4.22}$$

$$M_{12}(\omega,\omega) = M_{21}(\omega,\omega)^* = -\Gamma A(\omega)B(\omega)^* + (1/2)B(\omega)^*, \tag{4.23}$$

i.e.,

$$\alpha_+ + \alpha_- = (\Delta_1 - \Delta_N)\Gamma|B|^2, \tag{4.24}$$

$$\alpha_+\alpha_- = -\Delta_1\Delta_N|B|^2/4, \tag{4.25}$$

and for the CGF

$$\mu(\lambda) = -\frac{1}{2}\int \frac{d\omega}{2\pi}\ln\left[1 - 2\lambda(\Delta_1 - \Delta_N)\Gamma|B(\omega)|^2 - \lambda^2\Delta_1\Delta_N|B(\omega)|^2\right]. \tag{4.26}$$

Finally, inserting (2.8) and (2.9) the CGF can be expressed in the form

$$\mu(\lambda) = -\frac{1}{2}\int \frac{d\omega}{2\pi}\ln[1 + 4\Gamma^2|B(\omega)|^2 f(\lambda)], \tag{4.27}$$

where

$$B(\omega) = -i\omega G_{1N}(\omega), \tag{4.28}$$

$$f(\lambda) = T_1 T_N \lambda(-\lambda + 1/T_1 - 1/T_N). \tag{4.29}$$

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This expression is in agreement with Kundu et al. [3]. Here the form of $f(\lambda)$ ensures that the fluctuation theorem (4.5) holds. The deterministic dynamics of the chain is entirely embodied in the momentum Green's function $B(\omega)$.

V. DISCUSSION

Here we discuss four issues: i) the branch cut structure in $\mu(\lambda)$ and ensuing exponential tails in the heat distribution $P(Q/t)$, ii) a single bound Brownian particle coupled to two reservoirs, iii) a two particle chain coupled to heat reservoirs, and iv) an asymptotic expression for $\mu(\lambda)$ in the large N limit.

A. Exponential tails

By inspection of the general expression (4.27) for the CGF we infer that $\mu(\lambda)$ has the form of a downward convex function passing through the origin $\mu(0) = 0$ due to normalization and through $\mu(1/T_1 - 1/T_N) = 0$ owing to the fluctuation theorem. Since the argument in the log in (4.27) must be positive we infer the condition

$$f(\lambda) \geq -\frac{1}{4\Gamma^2 |B|_{\max}^2}, \tag{5.1}$$

where $|B|_{\max}$ is the maximum value of $|B(\omega)|$ in the ω range. By means of algebraic and trigonometric manipulations it can be shown that $|B(\omega)|^2$ is bounded by $1/4\Gamma^2$, for details see appendix A, and consequently, $f(\lambda) \geq -1$. By analyzing the expression for $f(\lambda)$ in (4.29) one easily finds that this bound is satisfied for $\lambda_- \leq \lambda \leq \lambda_+$, where the branch points $\lambda_\pm$ in $\mu(\lambda)$ are given by

$$\lambda_+ = 1/T_1, \tag{5.2}$$

$$\lambda_- = 1/T_N. \tag{5.3}$$

In Fig. 2 we have depicted the CGF given by (4.27) for the case $T_1 = 10$, $T_N = 12$, $\Gamma = 2$, $\kappa = 1$, and $N = 10$.

At large times the heat distribution function follows from (2.12), i.e.,

$$P(Q, t) = \int_{-i\infty}^{i\infty} \frac{d\lambda}{2\pi i} e^{-\lambda Q} e^{t\mu(\lambda)}, \tag{5.4}$$

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and the rate function or large deviation function $F(q)$ is given by

$$P(q) \sim e^{-tF(q)}, \tag{5.5}$$

$$q = \frac{Q}{t}. \tag{5.6}$$

Since $\mu(\lambda)$ is differentiable, strictly convex, and steep at the boundaries the Gärtner-Ellis theorem [37, 41] implies that the LDF is given by the Legendre transform

$$F(q) = \sup_\lambda \{q\lambda - \mu(\lambda)\}, \tag{5.7}$$

or

$$P(q,t) \sim e^{t(\mu(\lambda^*)-\lambda^* q)}, \tag{5.8}$$

where λ^* is determined by

$$\mu'(\lambda^*) = q, \tag{5.9}$$

and we find the LDF

$$F(q) = -\mu(\lambda^*) + \lambda^* \mu'(\lambda^*). \tag{5.10}$$

For $F(q)$ the fluctuation theorem has the form

$$F(q) - F(-q) = q(1/T_1 - 1/T_N). \tag{5.11}$$

Note that the LDF also follows from a heuristic saddle point argument, see [26]. In Fig. 3 we have depicted $-F(q)$ for the case $T_1 = 10$, $T_N = 12$, $\Gamma = 2$, $\kappa = 1$, and $N = 10$.

Replacing $\mu(\lambda)$ by the parabolic approximation

$$\mu_{\mathrm{par}}(\lambda) = \bar{q}\lambda(T_1 T_N \lambda + T_1 - T_N), \tag{5.12}$$

where $\bar{q}$ is given by (3.18) we obtain for $F(q)$

$$F_{\mathrm{par}}(q) = -\frac{(q - \bar{q})^2(T_1 - T_N)}{4\bar{q}T_1 T_N}, \tag{5.13}$$

in accordance with (5.11). For the heat distribution we obtain the displaced Gaussian $P(q) \propto \exp(-tF_{\mathrm{par}}(q))$; this also follows from general large deviation theory [37, 41].

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Deforming the contour in the integral (5.4) to pass along the real axis we pick up branch cut contributions in $\mu(\lambda)$. Heuristically, we conclude that for large $|q|$

$$F(q) \sim \lambda_+ q, \quad \text{for } q \gg 0 , \tag{5.14}$$

$$F(q) \sim |\lambda_-||q|, \text{ for } q \ll 0, \tag{5.15}$$

where λ_+ and λ_- have been defined above. This also follows directly form the Legendre transformation since $\mu(\lambda)$ is defined on a compact support. The linear behavior is confirmed by the plot of $F(q)$ for our particular choice of the parameter set, see Fig. 3. The heat distribution thus exhibits exponential tails for large $|q|$, i.e.,

$$P(q) \propto \exp(-\lambda_+ q t) \text{ for } q \gg 0, \tag{5.16}$$

$$P(q) \propto \exp(-|\lambda_-||q|t) \text{ for } q \ll 0, \tag{5.17}$$

with λ_+ and λ_- given by (5.2) and (5.3). It is interesting that the tails are determined only by the reservoir temperatures. Finally, we note that the exponential tails in $P(q)$ also follows from large deviation theory since μ is bounded by $\lambda_\pm$, see Refs. [37, 41].

B.   Bound Brownian particle

In an interesting paper Derrida and Brunet [4] considered a single Brownian particle driven by two reservoirs at distinct temperatures and presented an explicit expression for the CGF $\mu(\lambda)$. This toy model has also been discussed by Visco [53] who considered next leading term and the role of initial conditions; see also Farago [54].

In a previous paper [35] we considered an extension of this model to the case of a single particle attached harmonically to a substrate with spring constant κ using the simple method devised by Derrida and Brunet. We found that the CGF is *independent* of κ, indicating that the deterministic character of the spring does not influence the statistical properties of the long time heat transfer. Here we consider as an illustration the same problem within the present scheme and recover a CGF independent of κ. The configuration is shown in Fig. 4.

Associating the damping constants Γ_1 and Γ_2 with the two reservoirs the equation of motion take the form

$$\frac{du}{dt} = p, \tag{5.18}$$

$$\frac{dp}{dt} = -(\Gamma_1 + \Gamma_2)p - \kappa u + \xi_1 + \xi_2, \tag{5.19}$$

with noise correlations

$$\langle \xi_1(t)\xi_1(t')\rangle = 2\Gamma_1 T_1 \delta(t - t'), \tag{5.20}$$

$$\langle \xi_2(t)\xi_2(t')\rangle = 2\Gamma_2 T_2 \delta(t - t'). \tag{5.21}$$

In Fourier space we obtain the solution

$$p(\omega) = B(\omega)(\xi_1(\omega) + \xi_1(\omega)), \tag{5.22}$$

where

$$B(\omega) = \frac{-i\omega}{-\omega^2 + \kappa - i(\Gamma_1 + \Gamma_2)\omega}, \tag{5.23}$$

and

$$|B(\omega)|^2 = \frac{\omega^2}{(\omega^2 - \kappa)^2 + (\Gamma_1 + \Gamma_2)^2 \omega^2}; \tag{5.24}$$

note that $B(\omega)$ satisfies the Schwinger identity (3.28), i.e.,

$$B(\omega) + B(\omega)^* = 2(\Gamma_1 + \Gamma_2)|B(\omega)|^2. \tag{5.25}$$

The heat flux from the reservoir at temperature T_1 is

$$\frac{dQ}{dt} = p(-\Gamma_1 p + p\xi_1), \tag{5.26}$$

and we obtain from (5.22), (3.21), and (5.25) the diagonal matrix elements

$$M_{11}(\omega, \omega) = \quad \Gamma_2 |B(\omega)|^2, \tag{5.27}$$

$$M_{22}(\omega, \omega) = -\Gamma_1 |B(\omega)|^2, \tag{5.28}$$

$$M_{12}(\omega, \omega) = -\Gamma_1 |B(\omega)|^2 + (1/2)B(\omega)^*, \tag{5.29}$$

$$M_{21}(\omega, \omega) = -\Gamma_1 |B(\omega)|^2 + (1/2)B(\omega). \tag{5.30}$$

Following the prescription in Sec. IV the eigenvalue equation imply

$$\alpha_+ + \alpha_- = 2\Gamma_1\Gamma_2(T_1 - T_2)|B|^2, \tag{5.31}$$

$$\alpha_+\alpha_- = -\Gamma_1\Gamma_2 T_1 T_2 |B|^2, \tag{5.32}$$

and we obtain the CGF

$$\mu(\lambda) = -\frac{1}{2} \int \frac{d\omega}{2\pi} \ln\left[1 + 4\Gamma_1\Gamma_2 |B(\omega)|^2 f(\lambda)\right], \tag{5.33}$$

where $|B(\omega)|^2$ is given by (5.24) and $f(\lambda)$ by (4.29).

A straightforward evaluation of (5.33) using the integral [55]

$$\int \frac{d\omega}{2\pi} \ln\left(\frac{\omega^2 + a^2}{\omega^2 + b^2}\right) = a - b, \tag{5.34}$$

yields

$$\mu(\lambda) = (1/2)(a_+ + a_- - b_+ - b_-), \tag{5.35}$$

where

$$a_\pm^2 = (1/2)((\Gamma_1 + \Gamma_2)^2 - 2\kappa \pm \sqrt{((\Gamma_1 + \Gamma_2)^2 - 2\kappa)^2 - 4\kappa^2}, \tag{5.36}$$

$$b_\pm^2 = (1/2)(4\Gamma_1\Gamma_2 f(\lambda) + (\Gamma_1 + \Gamma_2)^2 - 2\kappa \pm \sqrt{(4\Gamma_1\Gamma_2 f(\lambda) + (\Gamma_1 + \Gamma_2)^2 - 2\kappa)^2 - 4\kappa^2}. \tag{5.37}$$

Further inspection shows, however, that the combination $a_+ + a_- - b_+ - b_-$ is *independent* of the spring constant κ, as already shown in [35], and we obtain

$$\mu(\lambda) = (1/2)\left[\Gamma_1 + \Gamma_2 - \sqrt{(\Gamma_1 + \Gamma_2)^2 + 4\Gamma_1\Gamma_2 f(\lambda)}\right]. \tag{5.38}$$

Introducing $f(\lambda)$, as defined in (4.29), we can express (5.38) in the form

$$\mu(\lambda) = \frac{\Gamma_1 + \Gamma_2}{2} - \sqrt{\Gamma_1\Gamma_2 T_1 T_2}\sqrt{(\lambda_+ - \lambda)(\lambda - \lambda_-)}, \tag{5.39}$$

where the branch points are given by

$$\lambda_\pm = \frac{1}{2}\left[1/T_1 - 1/T_2 \pm \sqrt{(1/T_1 - 1/T_2)^2 + (\Gamma_1 + \Gamma_2)^2/\Gamma_1\Gamma_2 T_1 T_2}\right]. \tag{5.40}$$

We note that $|B(\omega)|^2$ given by (5.24) has a two-peak structure with maximum value $1/(\Gamma_1 + \Gamma_2)^2$ at $\omega = \pm\sqrt{\kappa}$ and that the expressions (5.33) and (5.40) are in accordance with the general properties of $\mu(\lambda)$ discussed above. Finally, using (5.9) and (5.10) we obtain for the large deviation function $F(q)$,

$$F(q) = -(1/2)\left[\Gamma_1 + \Gamma_2 - q(\lambda_+ + \lambda_-) - (\lambda_+ - \lambda_-)\sqrt{\Gamma_1\Gamma_2 T_1 T_2 + q^2}\right], \tag{5.41}$$

which yields a heat distribution $P(q)$ in accordance with the general discussion in Sec. V A with exponential tails in the heat distribution; for more details regarding this model, see [35].

C. Two particle chain

As an illustration of the general scheme presented here we briefly consider the case of a chain composed of two particles; the configuration is depicted in Fig. 5. Setting $N = 2$ we have from (3.8), (3.14), and (3.27)

$$|B(\omega)|^2 = \frac{\kappa^2 \omega^2}{|\Omega(\omega)^2 - \kappa^2|^2}, \tag{5.42}$$

$$\Omega(\omega) = -\omega^2 + 2\kappa - i\Gamma\omega, \tag{5.43}$$

and we obtain from the general expression (4.27) the CGF

$$\mu(\lambda) = -\frac{1}{2} \int \frac{d\omega}{2\pi} \ln \left[1 + \frac{4\Gamma^2 \kappa^2 \omega^2 f(\lambda)}{|\Omega(\omega)^2 - \kappa^2|^2} \right]. \tag{5.44}$$

We have been unable to reduce the expression (5.44) further but note that for $\kappa = 0$ the LDF $\mu(\lambda) = 0$ for all λ, corresponding to two independent equilibrium systems at temperatures T_1 and T_2. We also remark that decoupling the chain from the walls, corresponding to setting $\Omega = -\omega^2 + \kappa - i\Gamma\omega$, we obtain $4\Gamma^2 \kappa^2 \omega^2 / (|\Omega^2 - \kappa^2|^2) = 4\Gamma^2 \kappa^2 / ((\omega^2 + \Gamma^2)|\omega^2 - 2\kappa + i\Gamma\omega|^2)$. In the limit of a stiff chain, corresponding to $\kappa \to \infty$, we have $4\Gamma^2 \kappa^2 \omega^2 / (|\Omega^2 - \kappa^2|^2) \to \Gamma^2 / (\omega^2 + \Gamma^2)$, i.e., the case of a single unbound particle coupled to two reservoirs, see Sec. V B.

D. N particle chain

In the limit of large N we present below an asymptotic expression for the CGF. For general N we have from (3.11), (3.14), (3.15), and (4.28)

$$|B(\omega)|^2 = \frac{4\kappa^3 \sin^2(p/2) \sin^2(p)}{|\Omega^2 \sin(N-1)p - 2\kappa\Omega \sin(N-2)p + \kappa^2 \sin(N-3)p|^2}, \tag{5.45}$$

which expanding the denominator can be expressed in the form

$$|B(\omega)|^2 = \frac{8\kappa^{-1} \sin^2(p/2) \sin^2(p)}{L(p) + K(p) \cos(2Np - \phi(p))}, \tag{5.46}$$

where

$$a = (1 - \alpha^2) \cos(p) - 2i\alpha, \tag{5.47}$$

$$b = (1 + \alpha^2) \sin(p), \tag{5.48}$$

$$L = |a|^2 + |b|^2, \tag{5.49}$$

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$$M = |b|^2 - |a|^2, \tag{5.50}$$

$$C = ab^* + a^*b, \tag{5.51}$$

$$K = \sqrt{M^2 + C^2}, \tag{5.52}$$

$$\alpha = (2\Gamma/\sqrt{\kappa})\sin(p/2), \tag{5.53}$$

$$\tan\phi = C/M. \tag{5.54}$$

By inspection we note that $|B(\omega)|^2$ displays an oscillatory structure with approximate period π/N, reflecting the resonance structure of the propagating lattice waves in the chain. The oscillations are modulated by the slowly varying functions of p, $\sin(p)$ and $\sin(p/2)$. Further inspection of (5.46) shows that the maxima are given by

$$|B(\omega)|^2_{\text{max}} = \frac{8\kappa^{-1}\sin^2(p/2)\sin^2(p)}{L(p) - K(p)}, \tag{5.55}$$

where a little analysis implies that $|B(\omega)|^2_{\text{max}}$ locks onto $1/4\Gamma^2$, corroborating the demonstration of the upper bound in appendix A. The lower bound of the oscillatory structure is, correspondingly, given by the envelope

$$|B(\omega)|^2_{\text{env}} = \frac{8\kappa^{-1}\sin^2(p/2)\sin^2(p)}{L(p) + K(p)}, \tag{5.56}$$

the structure is for $N = 10$ depicted in Fig. 9. The positions of the maxima and minima are given by the implicit conditions $2Np - \phi(p) = \pi \pmod{2\pi}$ and $2Np - \phi(p) = 0 \pmod{2\pi}$, respectively.

In p space, using $d\omega = \sqrt{\kappa}\cos(p/2)dp$, and inserting (5.46), the CGF given by (4.27) takes the form

$$\mu(\lambda) = -\int_0^\pi \frac{dp}{2\pi}\sqrt{\kappa}\cos(p/2)\ln\left[1 + \frac{16\Gamma^2\kappa^{-1}\sin^2(p/2)\sin^2(p)f(\lambda)}{L(p) + K(p)\cos(2Np - \phi(p))}\right]. \tag{5.57}$$

In the large N limit the rapid oscillations in $|B|^2$ allows us to integrate separately over each period. Using the integral [55], see also ref. [47],

$$\int_0^{2\pi} \frac{dp}{2\pi}\frac{1}{a + b\cos(p)} = \frac{1}{\sqrt{a^2 - b^2}}, \tag{5.58}$$

we thus obtain the following approximate form of $|B|^2$,

$$|B|^2_{\text{approx}} = \frac{8\kappa^{-1}\sin^2(p/2)\sin^2(p)}{\sqrt{L(p)^2 - K(p)^2}}. \tag{5.59}$$

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Further, inserting L and K from (5.49) and (5.52) we obtain

$$|B|^2_{\text{approx}} = \frac{2}{\Gamma\sqrt{\kappa}} \frac{\sin(p/2)\sin(p)}{1 + 4(\Gamma^2/\kappa)\sin^2(p/2)}, \tag{5.60}$$

and for the CGF in the limit $N \to \infty$

$$\mu(\lambda) = -\int_0^\pi \frac{dp}{2\pi} \sqrt{\kappa} \cos(p/2) \ln\left[1 + \frac{8\Gamma\kappa^{-1/2}\sin(p/2)\sin(p)f(\lambda)}{1 + 4(\Gamma^2/\kappa)\sin^2(p/2)}\right]. \tag{5.61}$$

In Fig. 6 we have for $N = 10$, $\Gamma = 2$, and $\kappa = 1$ depicted $|B|^2$, $|B|^2_{\max} = 1/4\Gamma^2$, $|B|^2_{\text{env}}$, and $|B|^2_{\text{approx}}$. We note that $|B|^2_{\text{approx}}$ smoothly interpolates over the oscillations in $|B|^2$. In Fig. 7 we depict $\mu(\lambda)$ as a function of μ for $N = 2$ and for $N = 10$. The other parameters are $\Gamma = 2$, $\kappa = 1$, $T_1 = 1$, and $T_N = 1$. We note the excellent fit already for $N = 10$ and the good approximation at small λ for $N = 2$.

The expression (5.61) for $\mu(\lambda)$ is manifestly independent of N in the large N limit. This implies according to (4.3) that the cumulants and in particular the mean current also are independent of N. This signals that Fourier's law is not valid for the harmonic chain, see e.g. ref. [36]. We also note that the large N limit does not correspond to the continuum limit; we just increase the number of particles in the chain keeping the lattice distance fixed.

VI.   GENERALIZED FLUCTUATION THEOREM

In Secs. IV and V we demonstrated the validity of the fluctuation theorem by an explicit evaluation of the CGF for the harmonic chain driven at the end points by heat reservoirs at distinct temperatures and considered, moreover, some special cases. Here we put these results in a more general framework by considering the Fokker-Planck equation for the characteristic function

$$C(\lambda, t) = \langle e^{\lambda Q(t)} \rangle. \tag{6.1}$$

For long times $C(\lambda, t) \sim \exp(t\mu(\lambda))$ and we obtain the differential equation

$$\frac{\partial C}{\partial t} = \mu(\lambda)C. \tag{6.2}$$

Expressing the Fokker-Planck equation for C in the form

$$\frac{\partial C}{\partial t} = L(\lambda)C, \tag{6.3}$$

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we identify the CGF $\mu(\lambda)$ as the maximal eigenvalue of the Fokker-Planck operator L. The issue is thus to establish the fluctuation theorem symmetry for the maximal eigenvalue.

We aim at a generalization of the fluctuation theorem to the case of many heat reservoirs, see also [4]. For that purpose we consider a setup where each particle in the chain couples to its own heat reservoir at temperature T_n. The configuration is depicted in Fig. 8. Generalizing (2.10) the heat flux to the n-th particle is given by

$$\frac{dQ_n}{dt} = p_n(-\Gamma p_n + \xi_n),\tag{6.4}$$

where the noise is correlated according to

$$\langle \xi_n(t)\xi_m(t')\rangle = 2\delta_{nm}\Gamma T_n\delta(t - t').\tag{6.5}$$

Since the transfer of heat induces a change in the state of the system we must at the outset consider the joint distribution $P(u, p, Q, t) \equiv P(\{u_n\}, \{p_n\}, \{Q_n\}, t)$. The heat distribution is then given by $P(Q, t) = \int \prod_n du_n dp_n P(u, p, Q, t)$.

As discussed in ref. [11], the Fokker-Planck equation for the joint distribution $P(u, p, Q, t)$ is derived by considering the heat $Q_n(t)$ as an independent dynamical variable, whose time evolution is governed by (6.4). Noting that the noise appearing in this equation is correlated to the noise appearing in the equation of motion for the momenta (2.2-2.5) one can write

$$\begin{aligned}\frac{\partial P}{\partial t} =& \quad \{P, H\} + \Gamma\sum_n\left(T_n\frac{\partial^2 P}{\partial p_n^2} + \frac{\partial}{\partial p_n}(p_n P)\right)\\ &+ \quad \Gamma\sum_n\left(\frac{\partial}{\partial Q_n}((p_n^2 + T_n)P) + T_n p_n^2\frac{\partial^2 P}{\partial Q_n} + 2T_n p_n\frac{\partial^2 P}{\partial Q_n\partial p_n}\right),\end{aligned}\tag{6.6}$$

where the Poisson bracket is given by

$$\{P, H\} = \sum_{n=1}^{N}\left[\frac{\partial P}{\partial p_n}\frac{\partial H}{\partial u_n} - \frac{\partial P}{\partial u_n}\frac{\partial H}{\partial p_n}\right];\tag{6.7}$$

see also ref. [26].

All reference to the deterministic dynamics of the chain is embodied in the Poisson bracket. The remaining terms in (6.6) are associated with the transfer of heat. Setting $\partial/\partial Q_n = -\lambda_n$ and $\partial^2/\partial Q_n^2 = \lambda_n^2$ we obtain for the characteristic function $C(u, p, \{\lambda_n\}, t)$ defined by the multiple Laplace transform [55]

$$P(u, p, \{Q_n\}, t) = \int_{-i\infty}^{i\infty}\prod_n\frac{d\lambda_n}{2\pi i}\exp(-\sum_n\lambda_n Q_n)C(u, p, \{\lambda_n\}, t),\tag{6.8}$$

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the Fokker-Planck equation (6.3), where the operator $L(\lambda)$ has the form

$$
\begin{aligned}
L(\lambda)C = \quad & \{C, H\} \\
+ \quad & \Gamma \sum_n \left[T_n \frac{\partial^2 C}{\partial p_n^2} + (1 - 2\lambda_n T_n) \frac{\partial}{\partial p_n}(p_n C) + (\lambda_n(\lambda_n T_n - 1)p_n^2 + \lambda_n T_n)C \right]. \quad (6.9)
\end{aligned}
$$

In the absence of coupling between the particles, i.e., for a vanishing Poisson bracket, $\{C, H\} = 0$, C is the characteristic function for the the heat transfers to N independent particles coupled individually to reservoirs at temperature T_n. Subject to the transformation $C = \exp(Et)\exp(g)\Psi$, where $g = (1/2)\sum_n(\lambda_n - 1/2T_n)p_n^2$, the Schroedinger-like equation $L\Psi = E\Psi$ describes N independent oscillators with spectrum $E = -\Gamma(n_1 + n_2 + \cdots n_N)$, $n_i = 0, 1, \cdots$. The maximal eigenvalue is given by $E = 0$ corresponding to $\mu = 0$, characteristic of an equilibrium configuration. Turning on the interaction between the particles the maximal eigenvalue will be shifted to a finite value and we obtain a nonvanishing λ-dependent CGF.

The structure of (6.9) also allows a simple derivation of a generalized fluctuation theorem; see also ref. [4]. The first step is to perform a "rotation" $\exp(H/T_m)$ with respect to the m-th reservoir in combination with a time reversal operator $\mathcal{T}$ and define the transformed Fokker-Planck operator

$$
\tilde{L}(\lambda) = e^{H/T_m}\mathcal{T}L(\lambda)\mathcal{T}^{-1}e^{-H/T_m}. \tag{6.10}
$$

In the next step we compare the operator $\tilde{L}$ with the adjoint operator L^*. Using $(\partial^2/\partial p_n^2)^* = \partial^2/\partial p_n^2$ and $(\partial p_n/\partial p_n)^* = -p_n\partial/\partial p_n$ and shifting the Laplace variables λ_n it turns out that $\tilde{L}$ and L^* become identical and we have the relationship

$$
\tilde{L}(\lambda) = L^*(\bar{\lambda}), \tag{6.11}
$$

where

$$
\bar{\lambda}_n + \lambda_n = 1/T_n - 1/T_m. \tag{6.12}
$$

Since $L(\lambda)$ is related to $\tilde{L}(\lambda)$ by a unitary transformation we infer that $L(\lambda)$ and $L^*(\bar{\lambda})$ have identical spectra and in particular identical maximal eigenvalues, i.e., the same large deviation function,

$$
\mu(\{\lambda_n\}) = \mu(\{\bar{\lambda}_n\}). \tag{6.13}
$$

The expression (6.13) together with (6.12) represents a generalization of the usual fluctuation theorem to many reservoirs. In the case of two reservoirs, setting $T_n = T_1$, $T_m = T_N$, and

$\lambda_n = \lambda$ we obtain the usual fluctuation theorem (4.5). We note that the above derivation holds for any time reversal invariant Hamiltonian, i.e., for any kind of interaction between the particles. In our derivation we have also assumed that the maximal eigenvalue is positive.

Thus, our proof of the fluctuation theorem is more general than the one given in Ref. [2], which is restricted to the harmonic chain only. Furthermore, our approach does not require a direct evaluation of the CGF, but is based only on the property of the dynamics, as expressed by the evolution operator $L(\lambda)$. The previous proof can be readily extended to the 3-D case, as long as $L(\lambda)$ has a form as in (6.9).

VII.   SUMMARY AND CONCLUSION

In this paper we have discussed a variety of issues regarding the noise driven harmonic chain. In Secs. III and IV we performed a calculation of the CGF, recovering the results of Kundu et al. [3], but adding some more details for the purpose of our analysis. In Sec V we discussed the exponential tails in the heat distribution, the bound single particle model, and the two-particle chain case. It is an interesting feature of the tails that the fall-off rate only depends on the noise features, i.e., the reservoir temperatures, and not on the dynamical properties of the chain such as the spring constant κ. In the large N limit we have found an analytical form for the CGF which excellently interpolates the exact result. This result is independent of N signalling that Fourier'r law does not hold. Finally, incorporating some of our results we have in Sec. VI within a Fokker-Planck description presented a generalization of fluctuation theorem to several reservoirs which holds for any interaction potential. The fluctuation theorem simply emerges from a symmetry hidden in the Fokker- Planck operator and is therefore not restricted to the linear chain but also holds for a 3D system.

Appendix A: Maxima of $|B(\omega)|^2$

Here we analyze the modulus squared of the function

$$B(\omega) = \frac{-i\omega\kappa \sin p}{D(\omega)}, \tag{A1}$$

where

$$D(\omega) = \Omega^2 \sin(N-1)p - 2\kappa\Omega \sin(N-2)p + \kappa^2 \sin(N-3)p, \tag{A2}$$

$$\Omega = -\omega^2 + 2\kappa - i\Gamma\omega, \tag{A3}$$

$$\omega^2 = 4k \sin^2(p/2), \tag{A4}$$

and demonstrate that it is bounded from above by $1/4\Gamma^2$, i.e., $|B(\omega)|^2 \leq 1/(4\Gamma^2)$.

Breaking up $|D(\omega)|$ in real and imaginary parts,

$$\Re\left[D(\omega)\right] = -4\kappa\Gamma^2 \sin^2(p/2) \sin(N-1)p + \kappa^2 \sin(N+1)p, \tag{A5}$$

$$\Im\left[D(\omega)\right] = -4\kappa^{3/2}\Gamma \sin(p/2) \sin Np, \tag{A6}$$

inserting $|B(\omega)|^2$, expressing ω in terms of p, using (A4), and substituting (A5)-(A6), we rephrase the condition $|B(p)|^2 \leq 1/(4\Gamma^2)$ as

$$g(p) = 16\kappa^3\Gamma^2 \sin^2(p/2) \left[\sin^2 Np - \sin^2 p\right]$$
$$+ (-4\kappa\Gamma^2 \sin(p/2) \sin(N-1)p + \kappa^2 \sin(N+1)p)^2 \geq 0. \tag{A7}$$

Expressing the $\sin(p/2)$ in terms of $\cos p$, and rearranging terms, $g(p)$ becomes

$$g(p) = k^2(-\Gamma^2 \sin Np + 2\Gamma^2 \sin(N-1)p - \Gamma^2 \sin(N-2)p + k \sin(N+1)p)^2, \tag{A8}$$

which is non negative thus demonstrating our assertion. The values of p for which $g(p) = 0$ correspond to the points of maximum for $|B(\omega)|^2$, with the exception of $p = 0, \pi$ where $D(\omega) = 0$. So, $|B(\omega)|^2$ has N-1 maxima where $|B(\omega)|^2 = 1/(4\Gamma^2)$, see Fig. 9.

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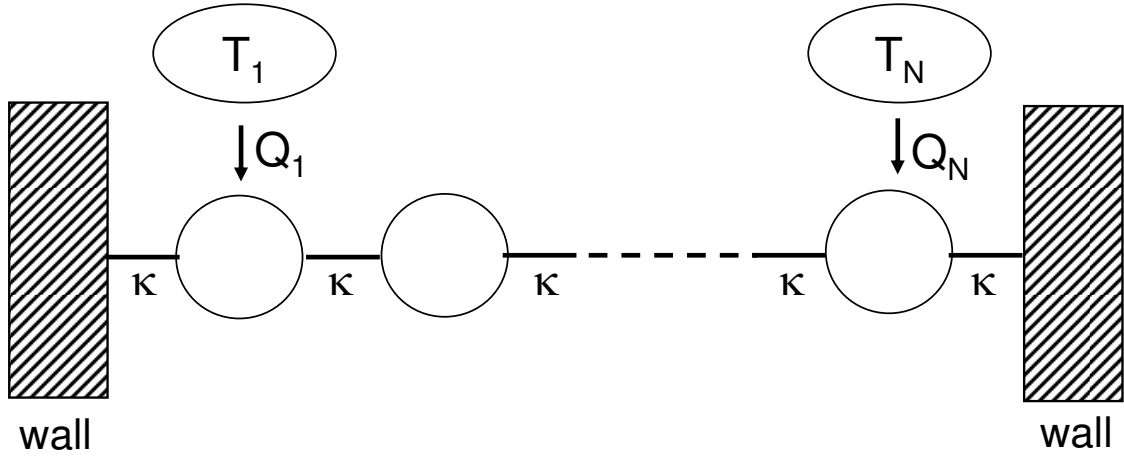[55] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals. Series, and Products* (Academic Press, New York, 1965).

FIG. 1: We depict a harmonic chain in contact with heat reservoirs at temperatures T_1 and T_N. The chain is attached to walls or substrates at the ends. The total heat transmitted to the $n = 1$ and $n = N$ particles are denoted Q_1 and Q_N, respectively. The spring constant is denoted κ.
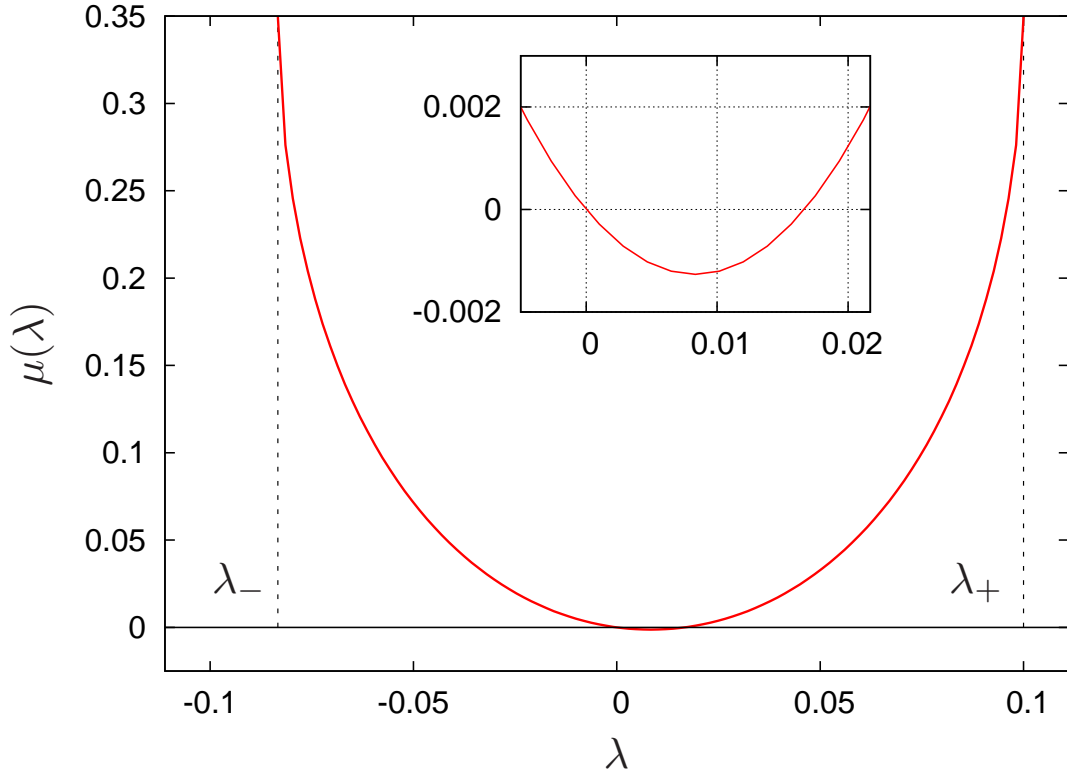

FIG. 2: Cumulant generating function $\mu(\lambda)$, as given by (4.27) for $T_1 = 10$, $T_N = 12$, $\Gamma = 2$, $\kappa = 1$, $N = 10$. Inset: zoom of the plot for small value of λ.
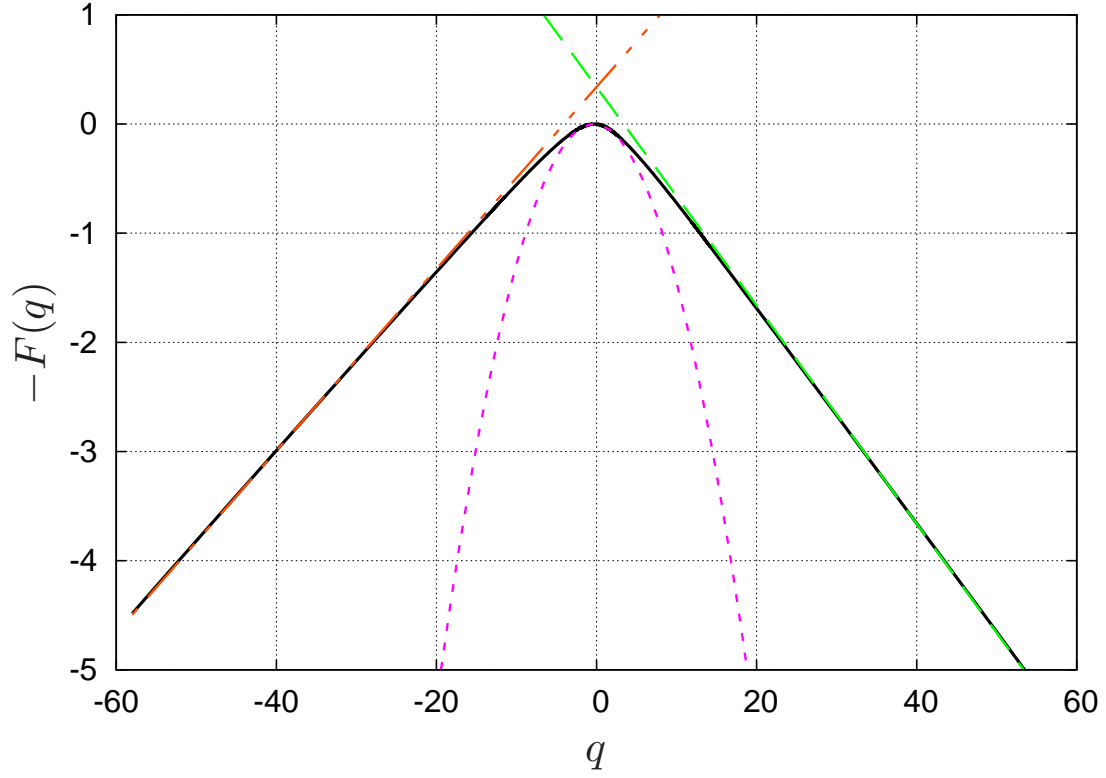
FIG. 3: Full line: plot of the large deviation function $-F$ as a function of q, as given by (5.10) for $T_1 = 10$, $T_N = 12$, $\Gamma = 2$, $\kappa = 1$, $N = 10$. Dotted line: parabolic approximation, (5.13). Dashed and dotted-dashed line: Linear regime for $|q| \gg \bar{q}$, the slopes are $-1/T_1$ and $1/T_N$, respectively.
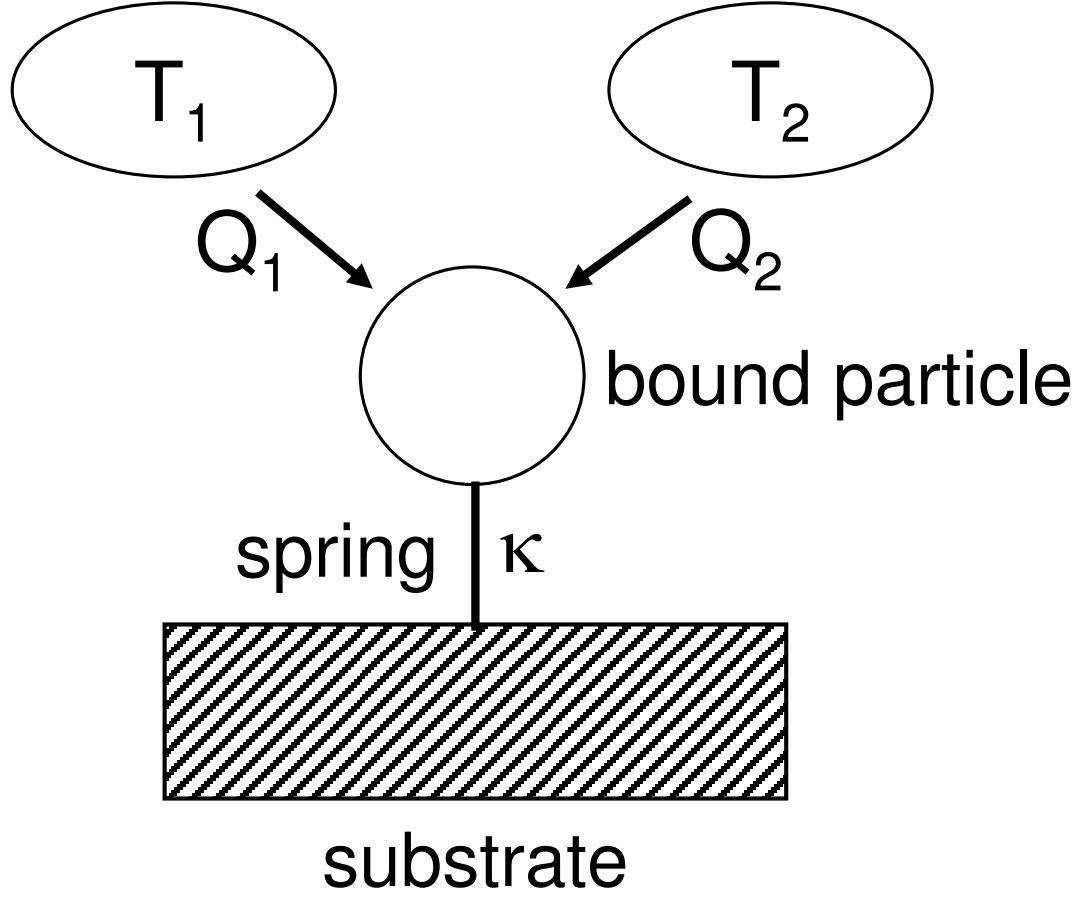
FIG. 4: We depict a harmonically bound particle interacting with heat reservoirs at temperatures T_1 and T_2. The heat transferred to the particle is denoted Q_1 and Q_2, respectively. The particle is attached to a substrate with a harmonic spring with force constant κ.
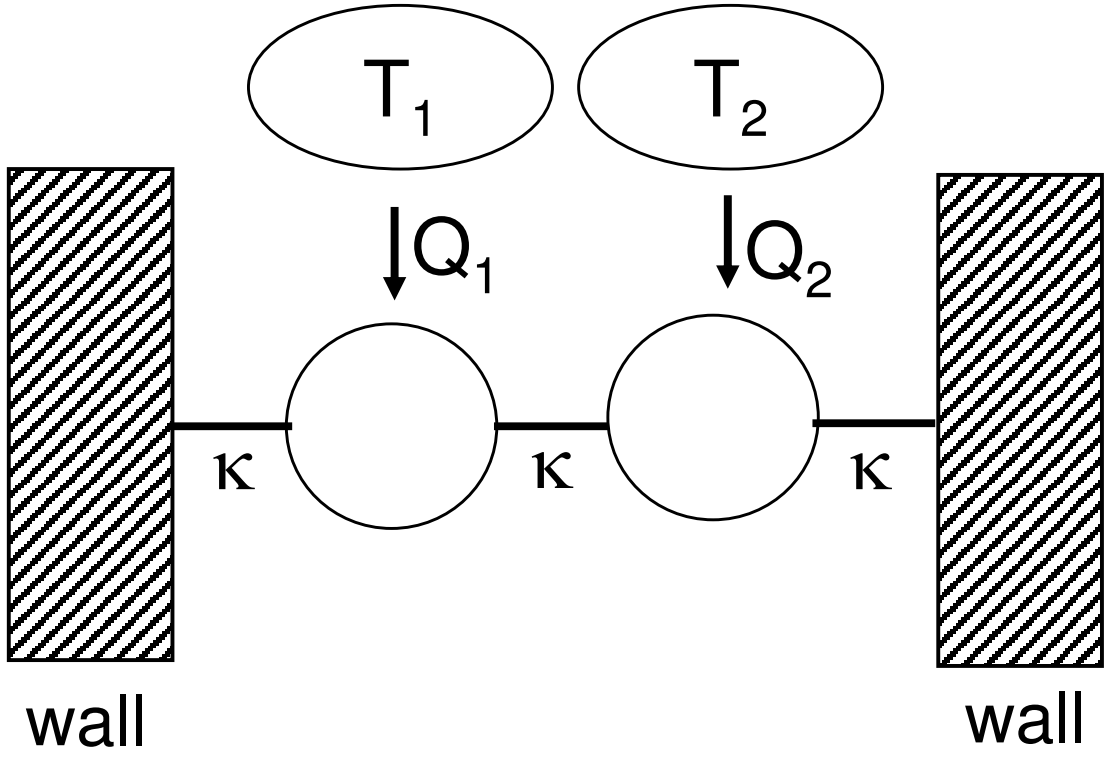
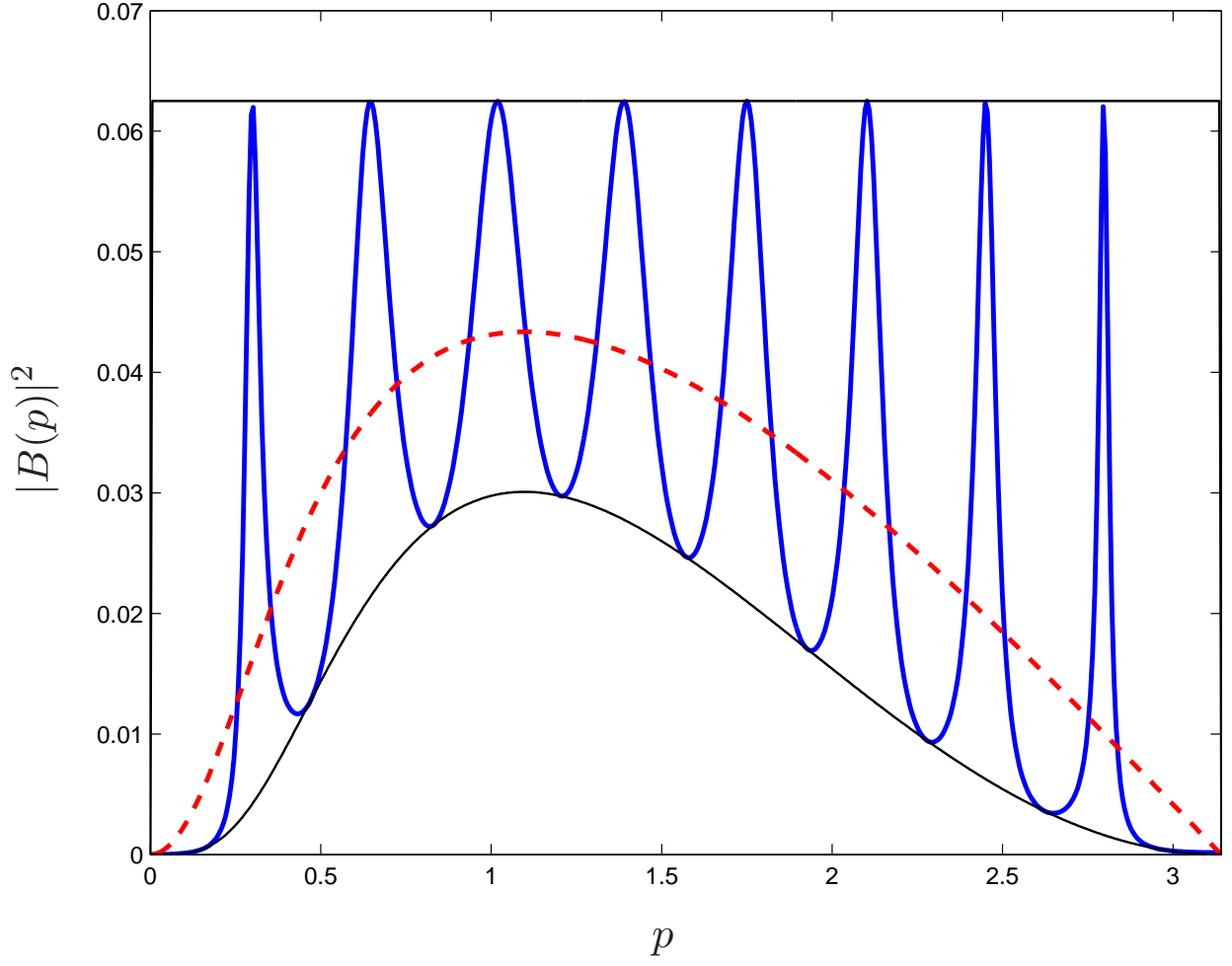FIG. 5: We depict a chain composed of two particles interacting with heat reservoirs at temperatures T_1 and T_2. The chain is attached to walls or substrates at the ends. The heat transferred to the particles is denoted Q_1 and Q_2, respectively. The particle is attached to a substrate with a harmonic spring with force constant κ.

FIG. 6: We depict the squared modulus $|B|^2$ given by (5.46) as function of p in the range $0 < p < \pi$ for $N = 10$, $\Gamma = 2$, and $\kappa = 1$ (blue). We also show the maximum value $|B|^2_{\max} = 1/4\Gamma^2$ (black) given by (5.55) , the envelope $|B|^2_{\mathrm{env}}$ (black) given by (5.56), and the large N approximation $|B|^2_{\mathrm{approx}}$ (red, dashed) given by (5.59).
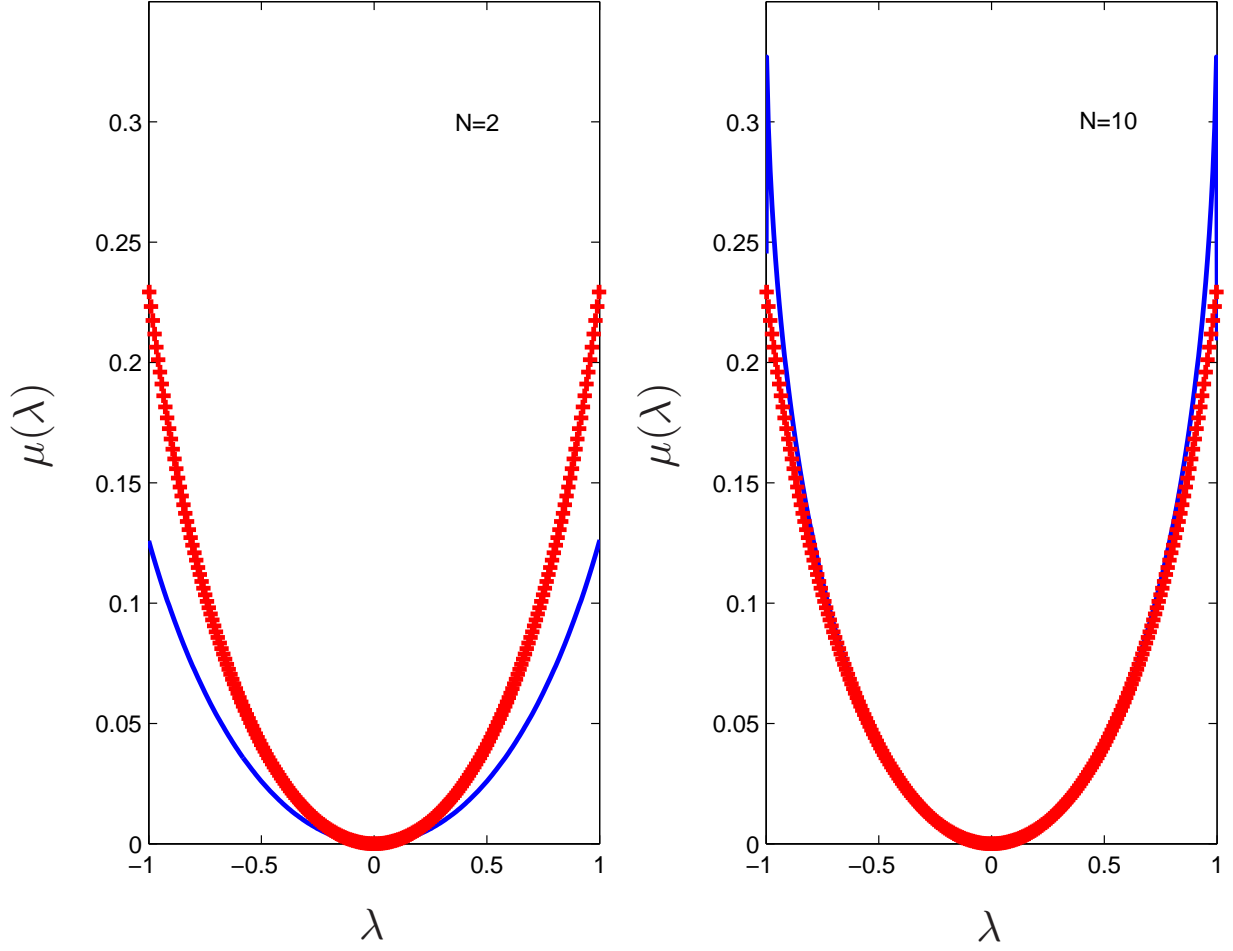
FIG. 7: We depict in two plots the LDF $\mu(\lambda)$ as a function of μ for $N = 2$ and $N = 10$, respectively. The parameters are $\Gamma = 2$, $\kappa = 1$, and $T_1 = T_N = 1$. The blue curve is based on the exact expression given by (5.57), the red plusses are given by the $N = \infty$ expression in (5.61).
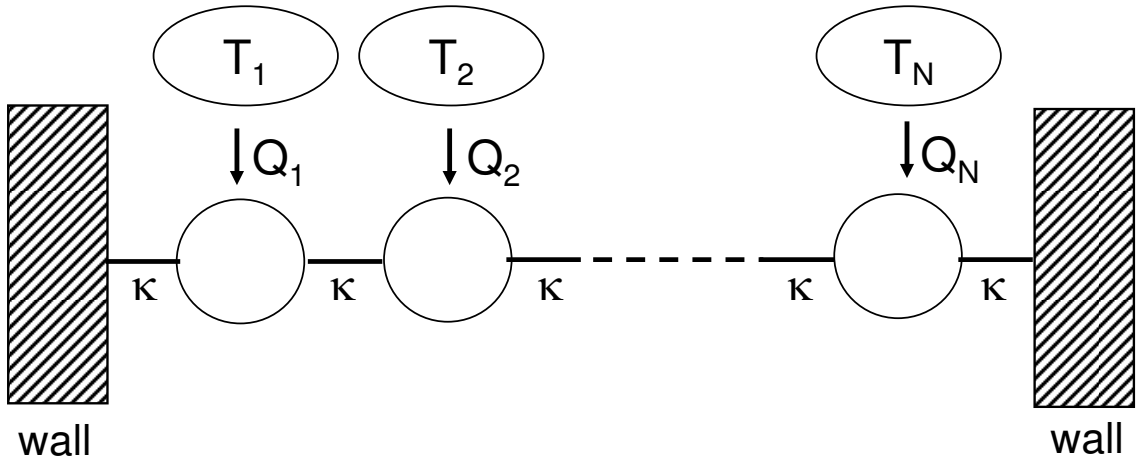
FIG. 8: We depict a harmonic chain where the n-th particle is in contact with a heat reservoir at temperatures T_n. The chain is attached to walls or substrates at the ends. The total heat transmitted to the n-th particle ise denoted Q_n The spring constant is denoted κ.
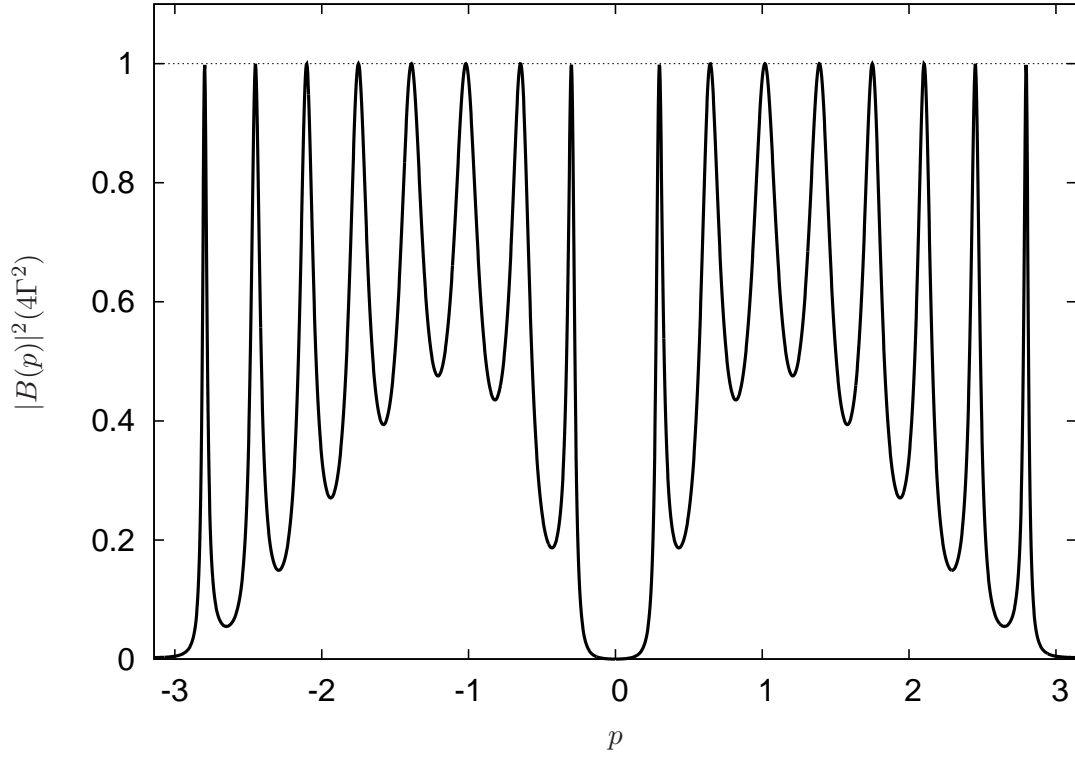

FIG. 9: Plot of the squared modulus of the momentum Green's function B as a function of p, as given by (A1) for $\Gamma = 2$, $\kappa = 1$, $N = 10$.